Non-local order in Mott insulators, Duality and Wilson Loops

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Abstract

It is shown that the Mott insulating and superfluid phases of bosons in an optical lattice may be distinguished by a non-local 'parity order parameter' which is directly accessible via single site resolution imaging. In one dimension, the lattice Bose model is dual to a classical interface roughening problem. We use known exact results from the latter to prove that the parity order parameter exhibits long range order in the Mott insulating phase, consistent with recent experiments by Endres et al. [Science **334**, 200 (2011)]. In two spatial dimensions, the parity order parameter can be expressed in terms of an equal time Wilson loop of a non-trivial $U(1)$ gauge theory in $2 + 1$ dimensions which exhibits a transition between a Coulomb and a confining phase. The negative logarithm of the parity order parameter obeys a perimeter law in the Mott insulator and is enhanced by a logarithmic factor in the superfluid.

Keywords: Mott insulators, optical lattices, non-local order, Wilson loops, duality

1. Introduction

A central assumption underlying both classical and quantum physics is that its basic laws are *local*, i.e., that the fundamental equations can be expressed in terms of relations between physical observables at a given point in space and time [1]. Symmetries and different types of order are thus related to the behavior of correlation functions of local observables. In particular, a qualitative change in macroscopic properties is typically associated with the appearance of long range order in some local observable $\hat{\mathcal{O}}(x)$. Its two-point correlation

$$\langle \hat{\mathcal{O}}(x)\hat{\mathcal{O}}(y)\rangle \to \mathcal{O}^2(\infty) \neq 0 \tag{1}$$

thus approaches a finite constant as $|x - y|$ goes to infinity. In recent years, a lot of interest has focussed on systems where this standard characterization of different phases of matter by finite values of some local order parameter $\hat{\mathcal{O}}(x)$ fails. This is the case, e.g., in the Quantum Hall Effect, a paradigmatic example of a topological insulator. It is an incompressible state described by a Chern-Simons theory which has gapless excitations associated with chiral edge currents [2, 3].

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Our aim in the present paper is to study non-local orders that may be used to characterize Mott insulating phases of lattice bosons. Quite generally, Mott insulators are defined by their incompressibility $\kappa = \partial n / \partial \mu \equiv 0$, a response function that is not associated with long range order in any local observable $\hat{\mathcal{O}}(x)$. Specifically, we focus on Mott insulators which do not break any lattice symmetries due to, for instance, the formation of a commensurate charge density wave [4] or due to Neel order in the spin degrees of freedom, as happens in Mott-Heisenberg insulators [5] realized in undoped high-temperature superconductors [6]. To investigate possible non-local orders that may exist in otherwise featureless Mott insulators, the particular case of bosons in an optical lattice is of special interest. By a simple change of the lattice depth, they may be tuned to undergo a superfluid (SF) to Mott insulator (MI) transition [7]. Moreover, thanks to the direct accessibility of the atomic distribution by optical imaging methods which allow measuring in situ density distributions [8] and even arbitrary density correlations at the single-atom level [9, 10], they also provide a new perspective on the microscopic details of the involved states. The question of whether some non-local order exists in the MI phase of bosons in an optical lattice has been addressed before by Berg et al. [11] in the particular case of one dimension. While their main focus has been the study of hidden 'string-order' that appears in the presence of repulsive interactions of finite range, they have shown via Bosonization that even in the much simpler situation of pure on-site repulsion, there is a non-local observable which takes finite values in the MI and is zero in the SF. Using single site imaging, the associated 'parity order parameter' (POP) has been measured by Endres et al. [12]. For lengths of up to eight lattice spacings their results were consistent with the theoretical expectation of a non-vanishing parity order in the MI and an algebraic decay to zero in the superfluid phase.

Our aim in the following is a detailed study of parity order in $d = 1$ and also in $d = 2$ dimensions using duality transformations. Specifically, in $d = 1$, a number of exact results for the parity order parameter are obtained from a systematic expansion around the atomic limit and from analytical results for the roughening transition of the equivalent classical interface model in two dimensions [13, 14, 15]. In the $d = 2$ case, the lattice bosons are dual to a three-dimensional $U(1)$ lattice gauge theory. This mapping has first been discussed by Peskin [16] starting from the classical three-dimensional XY model and has been extended to the two-dimensional quantum XY model by Fisher and Lee [17]. As will be shown here, the parity order parameter is mapped in the dual model on a quantity which is 'more local by one dimension': in $d = 1$, it is mapped on a two-point correlation function for a local operator of the type in Eq. (1) which shows an algebraic decay in the SF phase and converges to a constant in the MI. In the $d = 2$ case, the POP is mapped onto an equal time Wilson loop in the dual gauge theory, which serves to distinguish the superfluid and Mott insulating phases according to the dependence on the system size L. In particular, we find a perimeter law dependence in the MI phase which leads to an exponential decay of the POP while in the SF phase a logarithmic correction to the perimeter law leads to a super-exponential decay.

2. Bose-Hubbard Model and Parity Order

Ultracold bosons in an optical lattice provide a realization of the Bose-Hubbard model, as suggested theoretically by Jaksch et al. [18] and first realized experimentally by Greiner

et al. [7]. The associated many-body Hamiltonian [19]

$$\hat{H}_{\text{BH}} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right) , \qquad (2)$$

describes the competition between a kinetic energy which involves hopping to nearest neighbor lattice sites with amplitude $J > 0$ and an on-site repulsive interaction $U > 0$ which leads to an increase in energy if atoms hop to sites which are already occupied. Specifically, the operator $\hat{a}_i$ destroys a boson in a single particle Wannier state localized at lattice site i and the associated occupation number operator $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ has eigenvalues $0, 1, 2, \ldots$. We consider this model in both one and two spatial dimensions, specializing to the case of a simple quadratic lattice in the latter case. In either dimension, the ground state of the Bose Hubbard model exhibits a continuous transition between a superfluid and a Mott insulating state which may be tuned either by changing the ratio J/U at fixed density or by changing density at fixed J/U via the dimensionless chemical potential μ/U [19]. The universality class of this quantum phase transition is different in both cases. For the density driven Mott transition, the associated dynamical scaling exponent is $z = 2$ [20]. By contrast, changing the ratio J/U at fixed integer density $\bar{n} = 1, 2, \ldots$, the transition at the tip of the Mott lobes has $z = 1$, i.e., it is described by an $O(2)$-model in $D = d + 1$ dimensions which possesses a formal relativistic invariance [20]. It is this type of transition which will be considered in the following.

The superfluid phase of the Bose Hubbard model is characterized by a conventional, local observable $\hat{\mathcal{O}}(x) = \hat{a}_i$ associated with long range order in the one-particle density matrix, with $\mathcal{O}^2(\infty) \equiv n_0$ as the condensate density[1]. This order can be observed in a direct manner in time-of-flight images [7], which measure the momentum distribution as the Fourier transform of the one particle density matrix [21]. The excellent quantitative agreement between the measured absorption images after time-of-flight and precise quantum Monte Carlo calculations which include both the effects of finite temperature and the harmonic trap potential [22], shows that the Bose-Hubbard Hamiltonian (2) provides a faithful description of cold atoms in an optical lattice. In the Mott insulating phase, the correlation function of the local bosonic field operator vanishes exponentially like $\langle \hat{a}^\dagger(x) \hat{a}(0) \rangle \sim \exp(-|x|/\xi)$ with a correlation length $\xi \sim 1/\Delta$ that diverges like the inverse of the Mott gap Δ. The Mott phase is characterized by its incompressibility and has no associated order parameter, evolving in a continuous manner from a thermally disordered state as the temperature is lowered below the Mott gap Δ. Note that the observation of peaks in the noise correlations $\langle \hat{n}(\boldsymbol{x}) \hat{n}(\boldsymbol{x}') \rangle$ in the Mott phase after time–of–flight by Fölling et al. [23] does *not* reflect any long range order: they are a consequence of the fact that the Fourier components $\sum_{\boldsymbol{R}} n_{\boldsymbol{R}} \exp[i(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{R}]$ of the *average* density $n_{\boldsymbol{R}} = \langle \hat{n}_{\boldsymbol{R}} \rangle$ are of order N at wave vector differences $\boldsymbol{k} - \boldsymbol{k}' = m(\boldsymbol{x} - \boldsymbol{x}')/\hbar t$ which are equal to a reciprocal lattice vector $\boldsymbol{G}$.

As will be discussed in the following, the fundamental difference between the superfluid and Mott insulating phase in terms of their compressibility implies that there is

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[1]This would not be true if the bosons were charged as, e.g., the Cooper pairs of a conventional superconductor, where the role of $\hat{\mathcal{O}}(x)$ is expected to be taken by the bi-Fermion operator $\hat{\psi}_\uparrow \hat{\psi}_\downarrow (x)$. The associated correlation function $\langle \hat{\mathcal{O}}^\dagger(x) \hat{\mathcal{O}}(y) \rangle$, however, is not gauge invariant and therefore does not constitute a proper order parameter, as noted by Wen [2].

a non-local observable which behaves in a characteristically different manner in both phases. By a straightforward generalization of the parity order in 1d introduced by Berg et al. [11], the non-local order is defined as

$$\langle \mathcal{O}^2(\mathcal{D}) \rangle = \left\langle e^{i\pi \sum_{i \in \mathcal{D}}(\hat{n}_i - \bar{n})} \right\rangle = \left\langle \prod_{i \in \mathcal{D}}(-1)^{\bar{n}} \hat{p}_i \right\rangle , \qquad (3)$$

where $\mathcal{D}$ is a spatial domain, i.e., an interval in $d = 1$ and an area in $d = 2$, and $\hat{p}_i = (-1)^{\hat{n}_i}$ is the parity operator on lattice site i. There are two important properties of this observable which should be noted right away: First of all, the observable is easily accessible in experiments since, due to light-induced collision losses, quantum gas microscopes directly measure the on-site parity rather than the actual occupation numbers [10, 9]. As a second point, the observable must be calculated and measured in an *open* domain $\mathcal{D}$ which is part of a larger system, otherwise $\langle \mathcal{O}^2(\mathcal{D}) \rangle \equiv 1$ would trivially be equal to one due to conservation of particle number. To study the dependence on the size, we shall characterize the domain $\mathcal{D}$ by its linear extension L measured in units of the lattice spacing. In analogy to the standard definition (1) of long range order, the parity order parameter (POP) $\langle \mathcal{O}^2(L) \rangle$ exhibits long range order if $\langle \mathcal{O}^2(\infty) \rangle$ is finite.

This kind of order parameter is analogous to those studied in Ising models with a local gauge invariance, which have no conventional phase transitions to states with long range order, yet may exhibit different phases distinguished by non-local order parameters [24, 25, 26] (see also section 8). In the context of cold atoms, a more complicated 'string order' parameter was introduced, which characterizes a Haldane insulator that can form in one dimensional systems with longer range interactions [27]. Our focus is on the behavior of the parity order parameter at the conventional SF–MI transition, not only in 1d [11, 12] but also in 2d. In particular, we will use a duality transformation to show that in two dimensions parity order is related to an equal time Wilson loop in a non-trivial $U(1)$ gauge theory which exhibits different behavior as a function of system size L in the MI and SF phases.

3. Number fluctuations and area law

To obtain a qualitative understanding of the dependence of the non-local order defined in (3) on the size L of the domain we start by giving some qualitative arguments for the expected scaling behavior deep in the MI, where $J/U \ll 1$. Starting with the atomic limit, it is obvious that $\langle \mathcal{O}^2(L) \rangle|_{J=0} = 1$ in any dimension since particle fluctuations are then completely frozen. For small but finite J/U and for the simple case of a MI with average density $\bar{n} = 1$, particle number fluctuations appear as pairs of empty and doubly occupied sites. Now, for an arbitrary number of pairs which are completely inside the domain $\mathcal{D}$, the associated two minus signs in the product in Eq. (3) cancel. Only those pairs which are separated by the domain boundary lead to a reduction of $\langle \mathcal{O}^2(L) \rangle$ [12]. Intuitively one thus expects the parity order $\langle \mathcal{O}^2(L) \rangle \sim \exp(-L^{d-1})$ to scale exponentially with the area of the domain's boundary. This intuitive expectation is supported by a systematic perturbative calculation in an expansion around the atomic limit $J/U = 0$ which—as will be shown in section 4 below—yields

$$\langle \mathcal{O}^2(L) \rangle = 1 - 8\bar{n}(\bar{n} + 1)dL^{d-1}\left(\frac{J}{U}\right)^2 + \cdots \qquad (4)$$
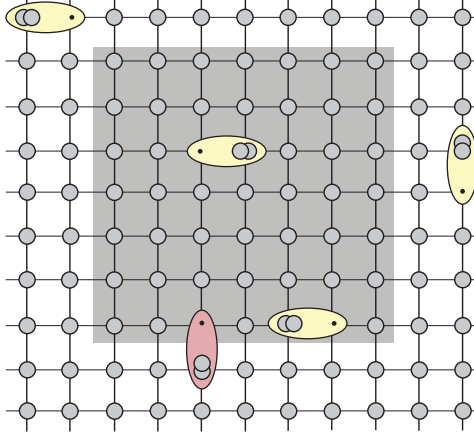
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Figure 1: (Color online) Illustration of how the order parameter is reduced from unity for $d = 2$. The grid lines indicate the lattice, bosons are represented by small circles. The domain $\mathcal{D}$, here taken to be a square, is shaded in gray. The minus signs from pairs which are completely inside or outside the domain (yellow ellipses) cancel out so that there is no contribution while pairs which are separated by the domain boundary (red ellipse) contribute a minus sign which leads to a reduction of $\langle \mathcal{O}^2(L) \rangle$.

up to second order in $J/U \ll 1$. Clearly the expansion is well defined only in $d = 1$, while in higher dimensions the effective expansion parameter $(J/U)^2 L^{d-1}$ is small only up to system sizes of order $(U/J)^{2/(d-1)}$.

Further insight into the origin of the perimeter law for the decay of the parity order can be gained by assuming that the expectation value in (3) may be calculated within a Gaussian approximation such that

$$\langle \mathcal{O}^2(L) \rangle \approx e^{\langle (i\pi \sum_{i \in \mathcal{D}} \delta \hat{n}_i)^2 \rangle / 2} = e^{-\pi^2 \langle \delta \hat{N}^2 \rangle / 2} \; , \tag{5}$$

where $\delta \hat{n}_i = \hat{n}_i - \bar{n}$. Within this approximation, $-\ln \langle \mathcal{O}^2(L) \rangle$ is simply a measure of the total number fluctuations $\langle \delta \hat{N}^2 \rangle$ in a domain of size L as part of an infinite system. Now, the standard thermodynamic relation $\langle \delta \hat{N}^2 \rangle = k_B T \, \partial N(\mu)/\partial \mu$ in this effectively grand canonical situation seems to indicate that these fluctuations vanish at zero temperature which would imply a trivial result $\langle \mathcal{O}^2(L) \rangle \equiv 1$ in the Gaussian approximation. This is not true, however, because the relation only applies in the thermodynamic limit and neglects boundary terms. For a careful calculation of $\langle \delta \hat{N}^2 \rangle$ at zero temperature and in a finite system, we generalize the analysis of Giorgini et al. ([28], see also [29, 30]) for Bose gases in a $d = 3$ continuum to arbitrary dimensions. The particle number fluctuations

$$\langle \delta \hat{N}^2 \rangle = S_d \int_0^{2L} \mathrm{d}r \, r^{d-1} \tau(r) \bar{n} \nu(r) \; , \tag{6}$$

in a spherical domain of radius L can then be calculated from the pair distribution function

$$\nu(\boldsymbol{r}) = \delta(\boldsymbol{r}) + n \left(g^{(2)}(\boldsymbol{r}) - 1 \right) = \int \frac{\mathrm{d}^d q}{(2\pi)^2} e^{i\boldsymbol{q} \cdot \boldsymbol{r}} S(\boldsymbol{q}) \tag{7}$$

and the volume $\tau(r)$ of the intersection between two d-dimensional balls of radius L separated by the distance r. Here, S_d is the surface of a unit sphere in d dimensions while $S(\boldsymbol{q})$ is the standard static structure factor.

In the superfluid, the zero temperature static structure factor has the non-analytic behavior $S(\boldsymbol{q}) \simeq \alpha|\boldsymbol{q}|$ at small wave numbers, characteristic for any compressible phase. Since collective excitations exhaust the f sum rule for long wavelengths, the prefactor $\alpha = \hbar/2mc_{\mathrm{s}}$ is, moreover, completely fixed by the exact sound velocity c_{s}. As a result of the non-analytic behavior of $S(\boldsymbol{q})$, the associated pair distribution function exhibits an algebraic decay $\nu(r) \simeq -\alpha/\pi r^2$ in $d = 1$ and $\nu(r) \simeq -\alpha/2\pi r^3$ in $d = 2$ at long distances. The behavior of the number fluctuations for large L is then found to be

$$\langle \delta N^2 \rangle \sim \alpha \bar{n} L^{d-1} \ln(L/\xi_{\mathrm{h}}) \quad (\mathrm{SF}) , \tag{8}$$

where the effective healing length $\xi_{\mathrm{h}} = \hbar/mc_{\mathrm{s}}$ serves as a short-distance cutoff. Within the Gaussian approximation, therefore, the parity order

$$\langle \mathcal{O}^2(L) \rangle \sim \begin{cases} L^{-\pi\alpha\bar{n}} & (d = 1) \\ L^{-\pi^2\alpha\bar{n}L} & (d = 2) \end{cases} \quad (\mathrm{SF}) \tag{9}$$

decays to zero with a power law in the superfluid phase in one dimension while in two dimensions, the decay is super-exponential.

In the MI phase, the quadratic number fluctuations are much smaller and the scaling of $\langle \delta N^2 \rangle$ with system size L differs in a qualitative manner from that in the SF. Indeed, at zero temperature, incompressibility of the MI implies that the structure factor vanishes analytically for $q \to 0$ and thus $S(\boldsymbol{q}) = \gamma(q\xi)^2 + \cdots$ to leading order in an expansion around $\boldsymbol{q} = 0$. Here, ξ is the characteristic length of the exponential decay of the one-particle density matrix mentioned in the previous section, while γ is a numerical constant which relates the scales appearing in the density correlation and in the one-particle density matrix. From perturbation theory, one finds that in one dimension γ is proportional to $(J/U)^2$ to leading order [31].

Since the static structure factor is analytic around $q = 0$, the pair correlation function $\nu(r)$ decays exponentially on the characteristic scale ξ, effectively cutting off the integral in Eq. (6). As a result, one finds that

$$\langle \delta N^2 \rangle \to bL^{d-1} \quad (\mathrm{MI}) \tag{10}$$

scales like the area of the boundary of the domain with a coefficient $b = b_0 \gamma \bar{n} \xi$, where b_0 is a numerical constant depending on the geometry and the precise functional form of $\nu(r/\xi)$.

The results obtained within this Gaussian approximation are—of course—not exact. Yet, as will be shown in sections 6 and 7 below, they give the correct qualitative behavior of the parity order parameter as a function of the size L of the domain. On a basic level, therefore, the different behavior of the non-local parity order in the MI and the SF is a simple consequence of the fundamental difference between number fluctuations in an incompressible versus a compressible system [32, 33]. In this context, it is also instructive to note that the underlying scaling $\langle \delta N^2 \rangle \sim \alpha \bar{n} L^{d-1} \ln(L/\xi)$ of the number fluctuations in the compressible and gapless superfluid compared to $\langle \delta N^2 \rangle \sim L^{d-1}$ in the incompressible and gapped MI are reminiscent of similar results obtained for the scaling

of the entanglement entropy $S(L)$. The fact that the fluctuations of conserved quantities are closely related to the latter, exhibiting a simple area law for gapped phases, has been noted by Swingle and Senthil [34]. There are, however, a number of important differences: the entanglement entropy typically scales like $S(L) = b\,L^{d-1}$ with a non-universal prefactor b even in gapless phases while the corresponding number fluctuations $\langle\delta N^2\rangle$ have an additional logarithmic enhancement factor for any phase with a finite compressibility. For the entanglement entropy, violations of the area law by a logarithmic factor of the form $S(L) \sim L^{d-1}\ln(L)$ appear, e.g., in free fermions with a Fermi surface and also for Landau Fermi liquids, not in a gapless superfluid, however. Indeed, as noted by Metlitski and Grover [35], its entanglement entropy $S(L) = b\,L^{d-1} + \Delta S$ exhibits an *additive*—not multiplicative—logarithmic contribution $\Delta S = \ln\left(\rho_{\mathrm{s}} L^{d-1}/c_{\mathrm{s}}\right)/2$ which is universal, i.e., it only depends on the superfluid stiffness ρ_{s} and the sound velocity c_{s} as effective low energy constants.

The simplicity of the Gaussian approximation for studying the parity order also allows for a straightforward discussion of how the above results are affected by a finite temperature. For a neutral SF, the structure factor at temperatures $k_B T \ll mc_{\mathrm{s}}^2$ reads [36] $S(\boldsymbol{q}) \simeq \alpha|\boldsymbol{q}|\coth(c_{\mathrm{s}}|\boldsymbol{q}|/2k_{\mathrm{B}}T)$. The characteristic length scale at which the zero temperature result $S(\boldsymbol{q}) \simeq \alpha|\boldsymbol{q}|$ is equal to the $q = 0$ thermal value $S(\boldsymbol{q} = 0) = 2k_{\mathrm{B}}T\alpha/c_{\mathrm{s}}$ is therefore given by $r_T = \hbar c_{\mathrm{s}}/2\pi k_{\mathrm{B}}T = \lambda_T^2/\xi_{\mathrm{h}}$, where λ_T is the thermal wavelength and $\xi_{\mathrm{h}} = \hbar/mc_{\mathrm{s}}$ the effective healing length. Since the parity order effectively probes number fluctuations at a finite wave vector $q \simeq 2\pi/L$ the zero temperature results remain valid as long as $r_T \gg L$. Since typical values of the healing length are of order $\xi_{\mathrm{h}} \sim 1\,\mu\mathrm{m}$, the characteristic scale of r_T becomes larger than a lattice spacing at temperatures below $T \approx 70\,\mathrm{nK}$.

An equivalent reasoning can be applied in the Mott insulating phase, where the thermal behavior of the structure factor $S(\boldsymbol{q} = 0) = \bar{n}k_{\mathrm{B}}T\kappa_T$ involves the compressiblity κ_T. For dimensional reasons, the latter must be of the form $\kappa_T = (\bar{n}\Delta)^{-1}f(\beta\Delta)$ with the Mott gap Δ and a function $f(\beta\Delta) \sim e^{-\beta\Delta}$ which has a thermally activated form. The zero temperature results are then valid as long as the domain size L satisfies

$$L \lesssim \lambda_T \xi \sqrt{\frac{m\Delta}{f(\beta\Delta)}}\,. \tag{11}$$

In the interesting regime $T \ll \Delta$ this is easily satisfied due to the exponential form of $f(\beta\Delta)$. The actual constraint is rather the condition $\beta\Delta \gg 1$ which becomes increasingly hard to satisfy as one approaches the critical point.

4. Perturbative analysis in the MI

Deep in the MI, where $J/U \ll 1$, exact results for the parity order can be obtained by a systematic perturbation theory around the atomic limit $J = 0$ of the Bose-Hubbard model. Here we make use of a method developed by van Dongen [37], which is an extension of a formalism due to Harris and Lange [38]. The basic idea is to construct a canonical transformation of the creation and annihilation operators, $\hat{a}^\dagger = e^{\hat{S}}\hat{b}^\dagger e^{-\hat{S}}$ with an anti-hermitian generator $\hat{S}$ such that in the new basis, the occupation numbers and hence the interaction part remain invariant under hopping. Explicitly, one writes

the Hamiltonian in the form $\hat{H} = U\hat{D} + \hat{K}$ and defines the hopping term for the new particles

$$\hat{T} = -J\sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j \quad \Leftrightarrow \quad \hat{K} = e^{\hat{S}}\hat{T}e^{-\hat{S}} \ . \tag{12}$$

The requirement that $\hat{D}$ is invariant under hopping is obeyed provided it is a constant of motion, i.e., $[\hat{H}, \hat{D}] = 0$. This condition fixes the transformation $\hat{S}$, which may be calculated order by order in a systematic expansion

$$\hat{S} = \sum_{n \geq 1} \frac{1}{U^n}\hat{S}_n, \tag{13}$$

in powers of $1/U$. By expanding the exponential and substituting the expansion of the operator $\hat{S}$, the POP takes the form

$$\langle \mathcal{O}^2(L) \rangle = 1 + e^{-i\pi N_0} \Bigg\{ \sum_k \frac{(i\pi)^k}{k!} \langle \Phi_0 | \left[\frac{1}{U}\hat{S}_1 + \frac{1}{U^2}\hat{S}_2 + \cdots , \left(\hat{N}(L) \right)^k \right] | \Phi_0 \rangle$$

$$+ \sum_k \frac{(i\pi)^k}{k!} \langle \Phi_0 | \frac{1}{2!} \left[\frac{1}{U}\hat{S}_1, \left[\frac{1}{U}\hat{S}_1, \left(\hat{N}(L) \right)^k \right] \right] | \Phi_0 \rangle + \cdots \Bigg\} \ , \tag{14}$$

where $\hat{N}(L)$ is the total number operator within the domain $\mathcal{D}$ and N_0 is the eigenvalue of $\hat{N}(L)$ in the atomic limit ground state $|\Phi_0\rangle$. Since $|\Phi_0\rangle$ is an eigenstate of $\hat{N}(L)$, the first term in the curly bracket vanishes at all orders. As a consequence, to calculate the POP at order n in J/U, one needs to determine the operators $\hat{S}_1, \ldots, \hat{S}_{n-1}$.

Specifically, substituting $\hat{S}_1$ from equation (A.1) (cf. Appendix A) and evaluating the commutators, one finds the result (4) stated already in section 3. In one dimension, we have continued the perturbative expansion up to fourth order in J/U. For reasons of space, the details of this calculation are deferred to Appendix A and we only give the result here:

$$\langle \mathcal{O}^2(L) \rangle = 1 - 8\bar{n}(\bar{n}+1)\left(\frac{J}{U} \right)^2 - \frac{4}{9}\bar{n}(\bar{n}+1)[\bar{n}(473\bar{n}+217) - 234]\left(\frac{J}{U} \right)^4 + \cdots \ . \tag{15}$$

Just as the leading order term, the next-to-leading correction is independent of the domain size L as long as the latter is larger than the order of perturbation. Hence, $\langle \mathcal{O}^2(L) \rangle$ is independent of L for sufficiently small J/U, in agreement with a DMRG calculation in [12] where $\langle \mathcal{O}^2(L) \rangle$ was found to be essentially independent of L for $J/U \lesssim 0.1$ for domain sizes ranging from 1 to 60.

5. Duality transformation

In the following, we show that within a reduced description of the SF to MI transition at fixed density in terms of a quantum rotor model [20], exact results for the parity order parameter can be obtained from analyzing a $(d+1)$-dimensional classical lattice model. This is particularly interesting in the $d = 2$ case where the parity order $\langle \mathcal{O}^2(L) \rangle$ can be expressed in terms of an equal time Wilson-loop in a nontrivial $U(1)$ gauge field which

is dual to the original lattice boson model. Our aim is twofold: first of all, unlike the qualitative arguments presented in section 3, the duality transformation permits us to derive exact results for the large L behavior of $\langle\mathcal{O}^2(L)\rangle$ in both the MI and SF phases within one unified framework. From a different point of view, however, the duality of the lattice boson model to a dynamical gauge field in $2+1$ dimensions can also be read the other way, where ultracold atoms in an optical lattice provide a quantum simulator of a nontrivial lattice gauge theory.

The starting point for the mapping is based on the realization that the SF to MI transition at fixed density is driven by phase fluctuations only [19]. To isolate these from the full Bose-Hubbard Hamiltonian, it is convenient to consider the limit of large filling $\bar{n} \gg 1$, where the boson operators may be rewritten in a density-phase representation, $\hat{a}_j \simeq e^{i\hat{\phi}_j}\sqrt{\bar{n}+\delta\hat{n}_j}$ [19]. In the limit $\bar{n} \gg 1$, the number fluctuations $\delta\hat{n}_j$ can be expanded up to second order and the Bose-Hubbard Hamiltonian is thus transformed into the Hamiltonian

$$H_{\mathrm{J}} = \frac{U}{2}\sum_{\boldsymbol{x}}\hat{n}_{\boldsymbol{x}}^2 + E_{\mathrm{J}}\sum_{\boldsymbol{x},\boldsymbol{u}}[1-\cos(\hat{\phi}_{\boldsymbol{x}+\boldsymbol{u}}-\hat{\phi}_{\boldsymbol{x}})] \tag{16}$$

of a system of quantum rotors at each lattice site $\boldsymbol{x}$ with a discrete eigenvalue spectrum $0,\pm 1,\pm 2,\ldots$ which are coupled to nearest neighbors $\boldsymbol{x}+\boldsymbol{u}$ by a Josephson energy $E_{\mathrm{J}} = 2\bar{n}J$. (Note that we have redefined $\delta\hat{n}_{\boldsymbol{x}} \to \hat{n}_{\boldsymbol{x}}$, i.e., $\hat{n}_{\boldsymbol{x}}$ is now the deviation from the average local occupation number).

Following a standard procedure, the partition function associated with the quantum rotor model (16) can now be expressed in terms of a path integral by dividing the interval $[0,\beta]$ into N_τ subintervals of width $\varepsilon = \beta/N_\tau$. Inserting a complete set of number states at each step, one thus obtains a discretized path integral representation of the form

$$Z_{\mathrm{J}} = \sum_{n_{\boldsymbol{x},j}\in\mathbb{Z}} \langle\{n_{\boldsymbol{x},1}\}|e^{-\varepsilon\hat{H}_{\mathrm{J}}}|\{n_{\boldsymbol{x},2}\}\rangle\cdots\langle\{n_{\boldsymbol{x},N_\tau}\}|e^{-\varepsilon\hat{H}_{\mathrm{J}}}|\{n_{\boldsymbol{x},1}\}\rangle\,, \tag{17}$$

where the notion $\{n_{\boldsymbol{x},j}\}$ is a reminder of the fact that—at given $j=1,\ldots,N_\tau$—there are N^d variables $n_{\boldsymbol{x},j}\in\mathbb{Z}$ for $\boldsymbol{x}\in(1,\ldots,N)^d$ that have to be summed over all integers $\mathbb{Z}$. In the limit $\varepsilon\to 0$, the non-commuting terms in $\exp(-\varepsilon\hat{H}_{\mathrm{J}})$ can be factorized to give

$$Z_{\mathrm{J}} = \sum_{n_{\boldsymbol{x},j}\in\mathbb{Z}}\prod_{\boldsymbol{x},j,\boldsymbol{u}}\left(e^{-\varepsilon U n_{\boldsymbol{x},j}^2/2}\langle\{n_{\boldsymbol{x},j}\}|e^{-\varepsilon E_{\mathrm{J}}[1-\cos(\hat{\phi}_{\boldsymbol{x}+\boldsymbol{u}}-\hat{\phi}_{\boldsymbol{x}})]}|\{n_{\boldsymbol{x},j+1}\}\rangle\right)\,. \tag{18}$$

The matrix elements of the Josephson coupling terms can now be simplified by using the so called Villain approximation[2] [39]

$$\exp\{-\varepsilon E_{\mathrm{J}}[1-\cos(\hat{\phi}_{\boldsymbol{x}+\boldsymbol{u}}-\hat{\phi}_{\boldsymbol{x}})]\} \simeq \sum_{m_{\boldsymbol{x},\boldsymbol{u}}}\exp\left(-\frac{m_{\boldsymbol{x},\boldsymbol{u}}^2}{2\varepsilon E_{\mathrm{J}}}-im_{\boldsymbol{x},\boldsymbol{u}}(\hat{\phi}_{\boldsymbol{x}+\boldsymbol{u}}-\hat{\phi}_{\boldsymbol{x}})\right)\,. \tag{19}$$

Since the fundamental symmetry $\phi\to\phi+2\pi$ due to the discreteness of the boson number is retained, this leaves the physics qualitatively unchanged. In one spatial dimension, this

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[2]a constant prefactor in (19) is suppressed because it only gives an irrelevant overall shift of the free energy.

approximation introduces one integer m_{lj} per lattice site, in two spatial dimensions, it introduces two integers $\boldsymbol{m}_{\boldsymbol{x},j} = (m_{\boldsymbol{x},x,j}, m_{\boldsymbol{x},y,j})$ at each lattice site.

For each given j, one now uses the fact that

$$\prod_{\boldsymbol{x}} \exp\left(-im_{\boldsymbol{x},\boldsymbol{u},j}(\hat{\phi}_{\boldsymbol{x}+\boldsymbol{u}} - \hat{\phi}_{\boldsymbol{u}})\right) = \prod_{\boldsymbol{x}} \exp\left(i(m_{\boldsymbol{x},\boldsymbol{u},j} - m_{\boldsymbol{x}-\boldsymbol{u},\boldsymbol{u},j})\hat{\phi}_{\boldsymbol{x}}\right) \tag{20}$$

for a periodic chain with $\hat{\phi}_{\boldsymbol{x}+N\boldsymbol{u}} = \hat{\phi}_{\boldsymbol{x}}$ and the identity $\langle n'|e^{im\hat{\phi}}|n\rangle = \delta_{n',n+m}$ since the operator $e^{im\hat{\phi}}$ shifts the particle number by m. The resulting partition function

$$Z_{\mathrm{J}} = \sum_{\substack{n_{\boldsymbol{x},j}\in\mathbb{Z} \\ m_{\boldsymbol{x},\boldsymbol{u},j}\in\mathbb{Z}}} \exp\left[-\frac{\varepsilon U}{2}\sum_{\boldsymbol{x},j} n_{\boldsymbol{x},j}^2 - \frac{1}{2\varepsilon E_{\mathrm{J}}}\sum_{\boldsymbol{x},\boldsymbol{u},j} m_{\boldsymbol{x},\boldsymbol{u},j}^2\right] \prod_{\boldsymbol{x},\boldsymbol{u},j} \delta_{\nabla_{\boldsymbol{x}}\cdot\boldsymbol{m}_{\boldsymbol{x},j},-\nabla_\tau n_{\boldsymbol{x},j}} \tag{21}$$

has a Gaussian form, however the variables $n_{\boldsymbol{x},j}$ and $\boldsymbol{m}_{\boldsymbol{x},j}$ are integer-valued and are connected by the constraint $\nabla_{\boldsymbol{x}}\cdot\boldsymbol{m} + \nabla_\tau n = 0$, where $\nabla_{\boldsymbol{x},\tau}$ denotes the discrete derivative on the dual lattice of links along the physical directions $\boldsymbol{x}$ and the 'time' direction τ. Thus, the variables $n_{\boldsymbol{x},j}$ and $\boldsymbol{m}_{\boldsymbol{x},j}$ together form a divergenceless $(d+1)$-dimensional integer vector field $\boldsymbol{n} \equiv (n,\boldsymbol{m})$. In $d=1$, this constraint may be resolved by introducing a single integer field $h_{x,\tau}$ such that $n = \nabla_x h$ and $m = -\nabla_\tau h$. The partition function then becomes that of the discrete Gaussian model with height variable h which describes the roughening transition of a 2d interface. Moreover, the POP is mapped on a two-point correlation function of the local variable $\mathcal{O}(x) = \exp(i\pi h(x))$. This model is discussed in section 6.

In $d=2$, the constraint is automatically satisfied if one introduces a three-component vector potential $\boldsymbol{a}$ such that $\boldsymbol{n} = \nabla \wedge \boldsymbol{a}$, where the lattice curl is defined as $(\nabla \wedge \boldsymbol{a}_{\boldsymbol{x}})_i = \sum_{j,k} \varepsilon_{ijk}(a_{\boldsymbol{x}-\hat{\boldsymbol{k}},k} - a_{\boldsymbol{x}-\hat{\boldsymbol{j}}-\hat{\boldsymbol{k}},k})$. The partition function then becomes that of a $(2+1)$-dimensional $U(1)$ gauge theory, as will be discussed in detail in section 7. Remarkably, under the duality transformation the parity order parameter is mapped onto an equal time Wilson loop [40]

$$\langle\mathcal{O}^2(L)\rangle = \left\langle\exp\left[i\pi\sum_{\boldsymbol{x}\in\mathcal{D}}\mathrm{d}^2 x\,(\nabla\wedge\boldsymbol{a})_\tau\right]\right\rangle = \left\langle\exp\left[i\pi\sum_{\boldsymbol{x}\in\partial\mathcal{D}}(\Delta\boldsymbol{x})\cdot\boldsymbol{a}\right]\right\rangle, \tag{22}$$

where we have used the discrete version of Stokes's theorem on the last line, $\partial\mathcal{D}$ is the boundary of the domain $\mathcal{D}$ and $\Delta\boldsymbol{x}$ is a unit vector directed along the boundary in the positive mathematical sense. The Wilson loop is a gauge-invariant quantity which is often used to characterize phases in gauge theories [41]. As will be shown in section 7, in the present case, the transition between a phase with massless and one with massive 'photons' in the underlying $U(1)$-gauge theory predicts qualitatively different behavior of the parity order in the SF and MI phases of the original lattice Boson model, consistent with the qualitative considerations discussed in section 3.

6. Discrete Gaussian interface model

As shown in the previous section, in the $d=1$ case the partition function can be represented in terms of a single integer h on each lattice site such that $(n,m) = (\nabla_x h, -\nabla_\tau h)$.

Choosing $\varepsilon = 1/U$,[3] the resulting partition function

$$Z_{\mathrm{DG}} = \sum_{\{h_{lj}\}} \exp\left[-\frac{1}{2}\sum_{l,j}\left\{(\nabla_x h_{lj})^2 + \frac{U}{E_{\mathrm{J}}}(\nabla_\tau h_{lj})^2\right\}\right] \qquad (23)$$

defines an anisotropic discrete Gaussian (DG) model for an integer valued height variable h_{lj} above a two-dimensional, perfectly flat interface $h_{lj} \equiv 0$ (note that an overall shift $h_{lj} \to h_{lj} + \mathbb{Z}$ of this reference plane is irrelevant). This mapping has been used earlier in the context of the SF-MI transition in one dimension by one of the present authors [42].

The DG model is a classical model which exhibits a phase transition from a smooth interface in the regime where U dominates to a rough phase in the limit $E_{\mathrm{J}} \gg U$. The smooth phase, which corresponds to the MI in the original quantum rotor model, is characterized by a finite dimensionless step free energy f_{s} [43] which is related to the Mott gap $\Delta\mu$ of the dual model (16) by $2f_{\mathrm{s}} = \Delta\mu/U$ [42]. The dimensionless step free energy is a decreasing function of E_{J}/U and reaches $f_{\mathrm{s}} \equiv 1/2$ at $E_{\mathrm{J}} = 0$. In this limit an additional boson is described by a step of unit height which is parallel to the τ axis, i.e., the boson world lines exhibit no quantum fluctuations.

When $E_{\mathrm{J}}/U \sim 1$, the model is essentially isotropic. To render this manifest, it is convenient to choose $\varepsilon = 1/\sqrt{E_{\mathrm{J}} U}$ so that

$$Z_{\mathrm{DG}} = \sum_{\{h_{lj}\}} \exp\left[-\frac{1}{2}\sqrt{\frac{U}{E_{\mathrm{J}}}}\sum_{l,j}\left\{(\nabla_x h_{lj})^2 + (\nabla_\tau h_{lj})^2\right\}\right] . \qquad (24)$$

In this representation, the ratio $\tilde{T}_{\mathrm{DG}} = \sqrt{E_{\mathrm{J}}/U}$ of kinetic and interaction energy in the underlying quantum rotor Hamiltonian (16) plays the role of an effective temperature. The discrete Gaussian model (24) is known to have a roughening transition of the Kosterlitz-Thouless type [44] at a critical temperature $\tilde{T}_{\mathrm{R}} \simeq 0.73$. In the smooth phase, the mean square surface displacement

$$\Delta h^2(L) = \langle (h_{lj} - h_{l'j'})^2 \rangle \qquad (25)$$

remains finite as the distance $L = |(l,j) - (l',j')|$ between two points on the surface approaches infinity. By contrast, the rough phase of the discrete Gaussian model at $\tilde{T}_{\mathrm{DG}} > \tilde{T}_{\mathrm{R}}$ is characterized by a logarithmically divergent $\Delta h^2(L) \sim \ln(L)$.

These results on the discrete Gaussian model, for which the existence of a Kosterlitz-Thouless transition has been proven rigorously by Fröhlich and Spencer [13], can now be translated back to understand the nature of non-local order in the original Bose-Hubbard or quantum rotor model. In particular, the qualitative results that were derived in section 3 within a Gaussian approximation from considering the number fluctuations within a domain of linear size L can now be put on a rigorous footing. This relies on the fact that number fluctuations in the original model of bosons hopping on a lattice are transformed, via the duality, to fluctuations of the normal vector of the 2d interface by

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[3]Note that the Trotter decomposition in Eq. (17) is usually performed for finite β and thus $N_\tau = \beta/\varepsilon \to \infty$ requires $\varepsilon \to 0$. Here we keep ε finite but consider the limit of zero temperature $\beta \to \infty$.

$n = \nabla_x h$. As a result, the nonlocal order parameter defined in Eq. (3) translates into the characteristic function

$$\langle \mathcal{O}^2(L) \rangle = \langle \exp(i\pi[h(L) - h(0)]) \rangle \tag{26}$$

of the probability distribution $p(h, |(l, j) - (l', j')|) = \langle \delta(h_{lj} - h_{l'j'} - h) \rangle$ that the height variables at two sites at a distance L differ by h.

For a detailed understanding of the behavior of the parity order parameter, we can now use exact results on the classical roughening transition of two-dimensional interfaces. Specifically, within the smooth phase, Forrester [14] has obtained the exact probability distribution for the height of a lattice site near the center in the body-centered solid-on solid (BCSOS) model for fixed boundary conditions and the thermodynamic limit: it turns out to be a discrete Gaussian distribution $p(h) = \mathcal{N}e^{-(h-1/2)^2/2\sigma^2}$, where $\mathcal{N}$ is a normalization constant, and with $\sigma^2 = C/\sqrt{1 - T/T_R}$ where $C = \sqrt{2/\ln 2}$. The non-zero expectation of this distribution stems from the fact that in the BCSOS model, one has to deal with two sublattices where the sites of one take only even values while the sites of the other take only odd values. Since the outermost sites are fixed at values 0 and 1 (according to the sublattice), the height in the center may equivalently be seen as the height *difference* to the border, or, in the thermodynamic limit, as the infinite-distance limit of this difference. Hence, the characteristic function of this probability distribution is just the two-point correlation function discussed above within the DG model. Since the DG and the BCSOS model are in the same universality class, we may conclude that in the limit of infinite distance, the probability distribution for the height difference between two points in the DG model equally becomes a discrete Gaussian distribution $p(\Delta h = n) = \mathcal{N}e^{-n^2/2\sigma^2}$ with[4] $\sigma^2 = C_{DG}/\sqrt{1 - \tilde{T}_{DG}/\tilde{T}_R}$. Using the Poisson formula, one then obtains the characteristic function

$$\sum_{n \in \mathbb{Z}} p(n)e^{ikn} = \frac{\sqrt{2\pi\sigma^2}}{\sum_{n \in \mathbb{Z}} e^{-n^2/2\sigma^2}} \sum_{m \in \mathbb{Z}} e^{-\sigma^2(k - 2\pi m)^2/2} , \tag{27}$$

i.e., the characteristic function is a periodic sum of Gaussians centered on $0, \pm 2\pi, \pm 4\pi, \ldots$. The prefactor is just the ratio of the normalization constants of the continuous and the discrete Gaussian distribution and tends to unity for $\sigma^2 \gg 1$. As $\tilde{T}_{DG}$ approaches $\tilde{T}_R$ from below, σ^2 diverges and the individual peaks of the characteristic function become very narrow. There are then only two contributions to the POP (from the peaks centered on 0 and 2π) which goes to zero as

$$\langle \mathcal{O}^2(\infty) \rangle = p(k = \pi) \sim 2 \exp\left(-\frac{\pi^2 C_{DG}}{2\sqrt{1 - \tilde{T}_{DG}/\tilde{T}_R}} \right) , \tag{28}$$

confirming the conjecture $\langle \mathcal{O}^2(L) \rangle \sim \exp\{-A[(J/U)_c - (J/U)]^{-1/2}\}$ made in [12] on how the POP reaches zero as one approaches the critical point from the smooth phase (close

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[4]Note that a priori, $C_{DG} \neq C$ [14]. The numerical values of the roughening temperatures are model-specific as well.

to the critical point, writing $\langle \mathcal{O}^2(L) \rangle$ as a function of J/U rather than $\tilde{T}_{\mathrm{DG}} \propto \sqrt{J/U}$ only affects the non-universal constant A).

To understand the behavior of the parity order within the superfluid, which corresponds to the rough phase of the associated 2d classical interface model, it is convenient to use the equivalence between the DG model and the classical two-dimensional Coulomb gas (CG) derived by Chui and Weeks [44]. Within the 2d CG picture, the underlying SF-MI transition is translated into a phase transition of the Kosterlitz-Thouless type between an insulating phase where charges are bound—the SF phase of the original model—and a metallic phase of effectively free charges which describes the MI. The metallic phase is characterized by a divergent polarizability $\int d^2r\, r^2 p(r)$, where $p(r)$ is the probability distribution function for the distance between a pair of opposite unit charges added to the system. Indeed, as shown by Chui and Weeks [44], for $0 < \xi < 2\pi$ the two-point correlation function of the DG model maps on the partition function of the Coulomb gas in the presence of two opposite charges $\pm\xi$ at a distance $r = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$,

$$\left\langle e^{i\xi[h(\boldsymbol{r}_1) - h(\boldsymbol{r}_2)]} \right\rangle = e^{-\beta_{\mathrm{CG}} F(r,\xi)} = p(r) \ , \tag{29}$$

where $F(r,\xi)$ is the free energy of the neutral Coulomb gas in the presence of the added charges. It is well known [45] that when these added charges have unit strength [within the mapping by Chui and Weeks, a unit charge corresponds to $\xi = 2\pi$ in $F(r,\xi)$],

$$e^{-\beta_{\mathrm{CG}} F(r,2\pi)} = \exp\left(-\frac{e^2}{\varepsilon_0} \ln r\right) = r^{-e^2/\varepsilon_0} \ , \tag{30}$$

with the dielectric constant ε_0 which characterizes the insulating phase of the Coulomb gas. At the unbinding transition, the polarizability diverges, i.e., the critical value of the dielectric constant obeys $(e^2/\varepsilon_0)_{\mathrm{c}} = 4$. In our case of $\xi = \pi$, we are dealing with a pair of half-unit charges[5]. As a result the POP

$$\langle \mathcal{O}^2(L) \rangle \sim r^{-e^2/4\varepsilon_0} \ , \tag{31}$$

decays algebraically in the SF phase of the original lattice Bose model, and the mapping to the Coulomb gas gives us the exact value of the universal jump of the exponent at the roughening temperature: for $\tilde{T}_{\mathrm{DG}} \to \tilde{T}_{\mathrm{R}}$ from above, the exponent $e^2/4\varepsilon_0$ approaches one before jumping to zero, a consequence of the universal jump of the superfluid stiffness at the SF-MI transition of the 1d quantum rotor model (for a more detailed discussion see [46]).

7. $U(1)$ gauge theory in $2 + 1$ dimensions

In $d = 2$, the duality mapping discussed in section 5 and the introduction of the three-component vector potential $\boldsymbol{a}$ with $\boldsymbol{n} = \nabla \wedge \boldsymbol{a}$ lead to a $(2+1)$-dimensional $U(1)$ gauge theory [2, 16, 17, 47, 48] (for an alternative approach to this type of duality mapping

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[5]To avoid possible confusion, we stress that the right-hand side of Eq. (29) is well-defined for arbitrary ξ, but the equality to the left-hand side (i.e., the existence of the mapping) is restricted to values $0 < \xi < 2\pi$, and thus to fractional charges. For $\xi = 2\pi n$ with integer n, one trivially has $e^{i\xi[h(\boldsymbol{r}_1) - h(\boldsymbol{r}_2)]} = 1$.

using the operator formalism, cf. [49]). Similarly to the 1d case, it is convenient to choose $\varepsilon = 1/\sqrt{UE_J}$, which results in a partition function of the form

$$Z = \sum_{\{a\}} \exp\left(-\frac{1}{2}\sqrt{\frac{U}{E_J}}\sum_{x,\tau}(\nabla \wedge a)^2\right) . \tag{32}$$

Since $(\nabla \wedge a)^2 = e^2 + b^2$ is the energy density associated with a two-component 'electric field' $e_i = \nabla_\tau a_i - \nabla_i a_\tau$ and a scalar 'magnetic field' $b = \nabla_x a_y - \nabla_y a_x$, this partition function appears to describe the free field theory of pure electrodynamics in $(2 + 1)$ dimensions [2]. It is gauge invariant since the action only depends on the curl of a and is thus unchanged if the lattice gradient of an arbitrary function of x and τ is added to a. What makes the model in Eq. (32) nontrivial is the fact that all fields take only integer values on a discrete space-time lattice. The SF to MI transition of the underlying lattice Bose model shows up at the level of the dual $U(1)$ gauge theory as a transition between a phase in which a really is a free field and the photon is massless and one with massive photons.

In order to understand the physical meaning of this transition in terms of the gauge field degrees of freedom, it is convenient to consider the equal-time one-body density matrix in the quantum rotor model (16), which is mapped onto a ratio of two gauge field partition functions

$$\frac{\langle \hat{a}^\dagger(\boldsymbol{x})\hat{a}\rangle}{\bar{n}} = \langle e^{i\hat{\phi}(\boldsymbol{x})}e^{-i\hat{\phi}(0)}\rangle = \frac{Z[\boldsymbol{x},0]}{Z} = \exp(-\Delta F[\boldsymbol{x},0]) , \tag{33}$$

where $Z[\boldsymbol{x},0]$ differs from Z in that the constraint $\nabla \cdot \boldsymbol{n}(\boldsymbol{y}) = 0$ is replaced by $\nabla \cdot \boldsymbol{n}(\boldsymbol{y}) = \delta_{\boldsymbol{y},\boldsymbol{x}} - \delta_{\boldsymbol{y},0}$ [50]. Physically, this corresponds to a configuration with a pair of oppositely charged magnetic monopoles situated at $\boldsymbol{x}$ and 0. The fact that the one-body density matrix approaches a constant in the SF and decays exponentially in the MI thus leads to a fundamentally different behavior of the dimensionless free energy increase

$$\Delta F[\boldsymbol{x},0] = \begin{cases} |\boldsymbol{x}|/\xi & \text{(MI)} \\ \text{const.} - \frac{c_s}{4\pi\rho_s|\boldsymbol{x}|} & \text{(SF)} \end{cases} \tag{34}$$

associated with the introduction of a monopole–antimonopole pair at distance $\boldsymbol{x}$ in the dual gauge theory (here, ρ_s and c_s denote the superfluid stiffness and sound velocity, respectively). In particular, the exponential decay of the one-body density matrix in the MI phase translates to a linear confinement while in the SF phase the monopoles interact via a 3d Coulomb potential.

An effective low energy description of the gauge theory which properly accounts for the two different phases is provided by a Gaussian model of the form

$$S = \frac{1}{2\tilde{T}} \int \mathrm{d}^3x \left\{[\nabla \wedge \boldsymbol{a}(\boldsymbol{x})]^2 + \frac{1}{\xi^2}[\boldsymbol{a}(\boldsymbol{x})]^2\right\} , \tag{35}$$

where $\boldsymbol{a}$ is now treated as a *continuous* variable and $\tilde{T} \simeq \sqrt{E_J/U}$ is a renormalized dimensionless temperature or coupling constant, similar to the one in the previous section. In the SF regime, where $\tilde{T}$ is above a critical value of order one, the gauge field is in

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its Coulomb phase where $\xi = \infty$. Elementary excitations are then massless photons, which are just the phonons of the superfluid with linear dispersion $\omega = c_{\mathrm{s}}|\boldsymbol{q}|$ (note that 'photons' in $(2+1)$-dimensional electrodynamics have no polarization degrees of freedom). By contrast, in the MI for small values of $\tilde{T}$, the gauge field is in a confining phase, with $\xi = 1/m$ finite. The photons thus acquire a mass m and now represent the elementary particle–hole excitations of the MI with dispersion $\omega = c_{\mathrm{s}}\sqrt{m^2 c_{\mathrm{s}}^2 + q^2}$ (at the transition, one has $c_{\mathrm{s}} = 4.8J$ for the Bose–Hubbard model with $\bar{n} = 1$ [51]). When evaluating expectations for the massless phase, it is convenient to keep a finite ξ during the calculation and only take the limit $\xi \to \infty$ at the end of the calculation, which avoids the necessity of introducing an explicit gauge-fixing term [52]. This can be seen explicitly in the correlation function of the vector potential, which reads

$$\langle a(\boldsymbol{q})_j a(\boldsymbol{q}')_k \rangle = \tilde{T}(2\pi)^3 \delta(\boldsymbol{q} + \boldsymbol{q}') \left[\frac{[P_t(\boldsymbol{q})]_{jk}}{\boldsymbol{q}^2 + \xi^{-2}} + \frac{[P_l(\boldsymbol{q})]_{jk}}{\xi^{-2}} \right] , \tag{36}$$

where $[P_t(\boldsymbol{q})]_{jk} = \delta_{jk} - q_j q_k / \boldsymbol{q}^2$ and $[P_l(\boldsymbol{q})]_{jk} = q_j q_k / \boldsymbol{q}^2$ are the components of the transverse and longitudinal projector with respect to $\boldsymbol{q}$, respectively. Since the effective model (35) is Gaussian, the calculation of the parity order parameter from the Wilson loop in Eq. (22) is now easy and gives[6]

$$\langle \mathcal{O}^2(L) \rangle = \exp \left(-\frac{\pi^2}{2} \left\langle \left(\int_{\mathcal{D}} \mathrm{d}^2 x \, [\nabla \wedge \boldsymbol{a}(\boldsymbol{x})]_\tau \right)^2 \right\rangle \right) . \tag{37}$$

Using (36), the expectation appearing in the exponent in Eq. (37) reduces to

$$\left\langle \left(\int_{\mathcal{D}} \mathrm{d}^2 x \, [\nabla \wedge \boldsymbol{a}(\boldsymbol{x})]_\tau \right)^2 \right\rangle = \tilde{T} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{q_x^2 + q_y^2}{\boldsymbol{q}^2 + \xi^{-2}} \left| \int_{\mathcal{D}} \mathrm{d}^2 x \, e^{i\boldsymbol{q}_\perp \cdot \boldsymbol{x}} \right|^2 , \tag{38}$$

where $\boldsymbol{q}_\perp = (q_x, q_y)$. Note that $\boldsymbol{q}$ has three finite components whereas $\boldsymbol{x}$ is restricted to the $\tau = 0$ plane. For a circular disk of radius R, the spatial integral appearing in (38) gives

$$\int_{\mathcal{D}} \mathrm{d}^2 x \, e^{i\boldsymbol{q}_\perp \cdot \boldsymbol{x}} = \frac{2\pi R}{q_\perp} \mathrm{J}_1(q_\perp R) . \tag{39}$$

In the deconfined phase, which corresponds to the superfluid, the mass parameter $1/\xi$ is equal to zero and the resulting parity order parameter is given by[7]

$$-\ln\langle \mathcal{O}^2(R) \rangle \sim \pi^3 \tilde{T} R \ln(\pi R) . \tag{40}$$

in agreement with the qualitative result obtained in Eq. (9) within the Gaussian approximation. Conversely, in the confined phase corresponding to the MI, The $\boldsymbol{q}^2$ is negligible compared with $1/\xi^2$, leading to a perimeter law

$$-\ln\langle \mathcal{O}^2(R) \rangle \sim \tilde{T}\xi^2 2\pi R \equiv \frac{R}{\ell_{\mathcal{O}}} . \tag{41}$$

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[6]The resulting scaling of the parity order will thus turn out to be the same as found in section 3 up to numerical factors, since both are obtained from a Gaussian model. Note, however, that the mapping of $\langle \mathcal{O}^2(L) \rangle$ to a Wilson loop in the dual gauge theory provides a proper justification for these scalings.

[7]The momentum integrals in (38) are cut off at $\Lambda \sim \pi$ since the original problem is defined on a lattice with lattice constant set equal to unity.

Thus, the characteristic decay length of the POP scales as $\ell_{\mathcal{O}} \sim \Delta^2 \sqrt{U/J}$ close to the critical point. Remarkably, a measurement of the parity order, which only involves the statistics of number fluctuations, therefore allows to extract the Mott gap.

8. Conclusion & Outlook

We have presented a detailed study of parity order $\langle \mathcal{O}^2(L) \rangle$ for lattice bosons in both one and two spatial dimensions, using duality transformations. Consistent with previous theoretical work [11] and recent experiments [12], it has been shown that the Mott insulating phase in one dimension exhibits long range parity order. An intuitive understanding of this result relies on the observation that for any incompressible phase, the number fluctuations $\langle \delta \hat{N}^2 \rangle \sim L^{d-1}$ in a domain of size L scale with the area of the boundary $\sim L^{d-1}$. Using the duality to a discrete, classical interface roughening problem in two dimensions, these results have been put on a rigorous footing. In two dimensions, the parity order again shows qualitatively distinct behavior in the MI and SF phase. In this case, the variable $\langle \mathcal{O}^2(L) \rangle$ can be expressed in terms of an equal time Wilson loop of a nontrivial $U(1)$ gauge theory in $2+1$ dimensions. This is related to the fact that the density fluctuations in the original lattice Bose model are mapped to the scalar magnetic field in the dual gauge theory. A quite interesting result obtained from this mapping is the fact that the decay of parity order in the MI allows to measure the Mott gap from the statistics of number fluctuations. Since experimental measurements of the parity order in two dimensions are straightforward in principle, this seems a promising route to infer microscopic information from single site resolution imaging which is very difficult to obtain otherwise. The detailed numerical factors in the scaling of $\langle \mathcal{O}^2(L) \rangle$ can unfortunately not be predicted from our effective long wavelength description of the quantum rotor model. Since we are dealing with a bosonic system, however, effective numerical methods are available to obtain precise results in a realistic experimental setup, as has been shown for thermodynamic properties and excitation energies [51]. In particular, numerical simulations directly deal with the Bose Hubbard model which applies in the relevant case of low filling $\bar{n} = 1$ instead of the qualitatively similar situation $\bar{n} \gg 1$ that has been studied here within the quantum rotor model.

An important open question is, of course, to which extent our results for Bose Mott insulators can be generalized to the fermionic case, which has also been realized experimentally with ultracold atoms [53, 54]. Based on the qualitative description in terms of the scaling of number fluctuations in section 3, we expect that the results obtained here carry over to the fermionic case despite the fact that no duality transformations exist in this case which allow to connect the parity order with a Wilson loop in a dual gauge theory. The presence of long range parity order for 1d Mott insulators also in the fermionic case is consistent with the results of a recent DMRG study of the fermionic Hubbard model by Montorsi and Roncaglia [55]. A different kind of non-local order characterized by sub-lattice parity was found in this Model by Kruis et al. several years earlier [56, 57].

Finally, a quite interesting direction of further research on non-local orders for cold atoms in optical lattices is connected with the recent realization of a 1d transverse Ising model using a tilted optical lattice [58]. Extending this setup to the case of two dimensions, a number of complex phases may appear depending on the type of lattice and the direction of the tilt [59]. A quite intriguing perspective would appear in a setup that

allows to realize a ferromagnetic version of this standard model for quantum phase transitions [20]. In the ferromagnetic case, the transverse Ising model is self-dual in one dimension, while in two dimensions the dual theory is given by an Ising gauge theory [41]. For the latter, one can define non-local correlation functions as $C(\mathcal{D}) = \langle \prod_{m \in \mathcal{D}} \hat{S}_m^x \rangle$, where $\hat{S}_m^x$ is the x component of the spin operator at site m and $\mathcal{D}$ is an area in two dimensions, in complete analogy with our definition of the parity order in equation (3). After the duality transformation, this observable is transformed into $C(\mathcal{D}) = \langle \prod_{k \in \partial \mathcal{D}} \hat{\sigma}_k^z \rangle$, where $\hat{\sigma}_k^z$ is the z component of the spin operator at site k in the dual theory and $\partial \mathcal{D}$ are the two sites at both ends of the string in one dimension or the border of the area in two dimensions. As a result, one has in one dimension that $\lim_{L \to \infty} C(L) > 0$ for the paramagnetic phase. In two dimensions, $C(\mathcal{D})$ is a Wilson-Wegner loop around a closed path [24, 41], which shows an exponential scaling with the perimeter of the loop in the paramagnetic phase and with the enclosed area in the ferromagnetic phase of the original model [41, 60]. However, the detection of the non-local order parameter requires the measurement of the x component of the spin operator, which in turn requires the single-site resolved detection of the phase coherence between superposition states with different on-site occupation numbers, a technique that is so far not available.

Acknowledgements

Appendix A. Details about the perturbative calculation

According to the program outlined in Section 4, calculting the POP to nth order in J/U amounts to calculating the operators $\hat{S}_1, \ldots, \hat{S}_{n-1}$. Hence, for the second order result, we only need to calculate one operator. One finds

$$\hat{S}_1 = \sum_{D_1, D_2}{}' \frac{1}{D_2 - D_1} \hat{P}_{D_2} \hat{T} \hat{P}_{D_1} , \tag{A.1}$$

where the sums go over the eigenvalues D of the operator $\hat{D}$ and $\hat{P}_D$ is the projector on the eigenspace corresponding to this eigenvalue. Moreover, here and in the following, a prime on a sum indicates that values which make the denominator vanish are excluded from the sum.

One may imagine the calculation of the expectation $\langle \mathcal{O}^2(L) \rangle$ as summing over all possible hopping processes where the order in J/U indicates the number of occurring hops. For example, at second order, starting from a situation with uniform filling corresponding to $|\Phi_0\rangle$, all possible processes consist of a single particle hopping to a neighboring site and back again. Different contributions stem from the position of the starting lattice site and its neighbor relative to the domain boundary and from the position of the operator $\hat{N}(\mathcal{D})$ in the product of operators.

The next non-vanishing contribution to the POP is of fourth order, so we need to calculate $\hat{S}_{2,3}$. The former turns out to be given by

$$\hat{S}_2 = \sum_{D_1,D_2,D_3}{}' \frac{1}{2\left(D_2 - D_1\right)} \left(\frac{1}{D_2 - D_3} - \frac{1}{D_3 - D_1} \right) \hat{P}_{D_2} \hat{T} \hat{P}_{D_3} \hat{T} \hat{P}_{D_1}$$

$$+ \sum_{D_1,D_2}{}' \frac{1}{\left(D_2 - D_1\right)^2} \left(\hat{P}_{D_2} \hat{T} \hat{P}_{D_1} \hat{T} \hat{P}_{D_1} - \hat{P}_{D_2} \hat{T} \hat{P}_{D_2} \hat{T} \hat{P}_{D_1} \right) . \quad \text{(A.2)}$$

The expression for $\hat{S}_3$ is too unwieldy to reproduce here, so we limit ourselves to a description of the involved hopping processes. They can be grouped into four types:

- Back- and forth hoppings of two particles separated by more than two lattice sites, i.e., independent second order processes.

- Processes where the same particle or hole hops twice before returning to its original site.

- Processes where a particle hops twice and is then followed by the created hole or vice versa.

- Processes where two particles start or end on the same lattice site before hopping back (cf. Fig. A.2).
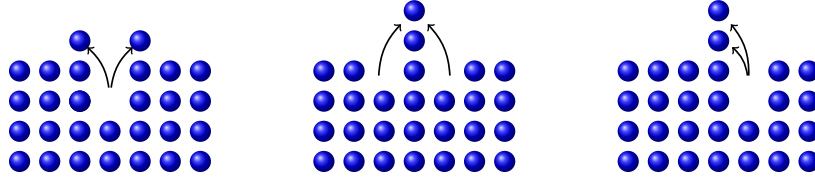

Figure A.2: (Color online) Possible processes at fourth order where two particles start or end on the same lattice site. The images show the configuration after two hopping events (the remaining two restore uniform filling) for $\bar{n} = 4$.

Summing over all contributions finally yields Eq. (15).

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